Cylindrical Ion Trap Mass Spectrometer for Chemical Warfare Agent Detection and Identification

M. Todd Griffin, Jack E. Fulton, Jr., Robert F. McAtee,
Norm Popkie, Michael A. Eagan, Mike Jahn

Night Vision/Electro Optics and Chemical/Biological/Explosives Detection Group
Naval Surface Warfare Center, Crane Division
Crane, IN 47522

Rong Gao, Lefteri H. Tsoukalas, R. Graham Cooks
Purdue University
W. Lafayette, IN 47907-1290

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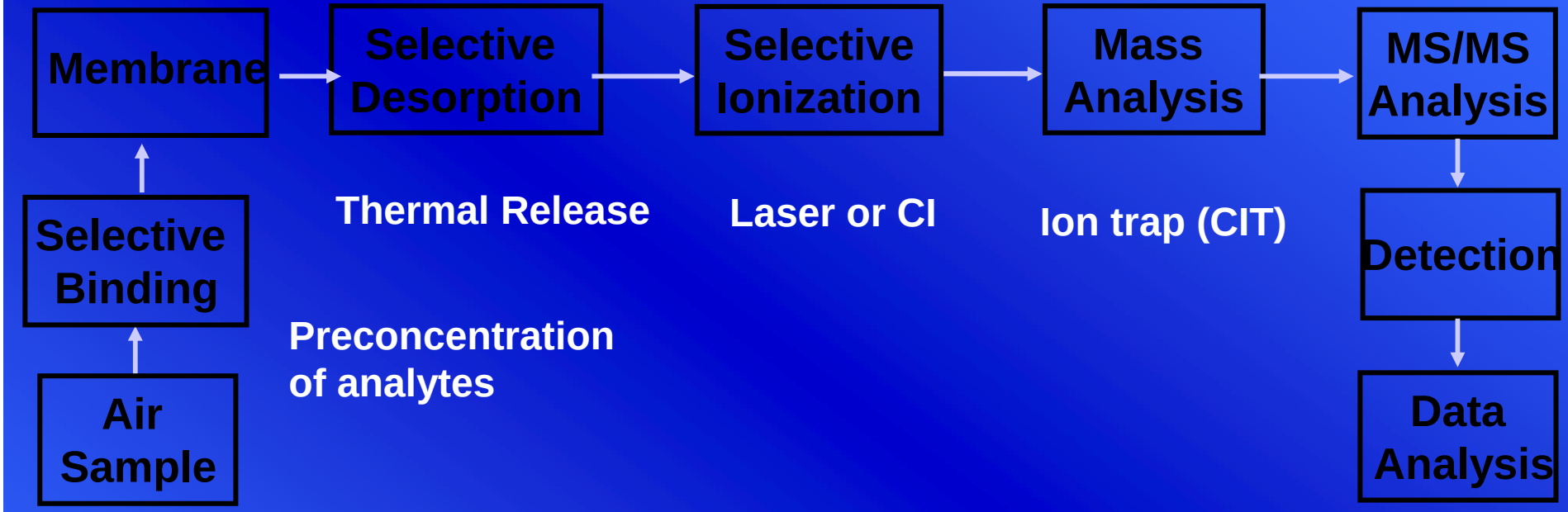
Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

Selective, Rapid Detection of Chemical Warfare Agents in Air by Ion Trap Mass Spectrometry

- **Requirements, field portable plus**
  - **Speed of analysis:** < 10 seconds
  - **Sensitivity:** LOD < 1 part per trillion by volume
  - **Selectivity:** samples are complex mixtures of organics
- **The Solution**
  - Miniature mass spectrometer
  - Ion trap with simple cylindrical electrodes
  - Rapid, selective membrane introduction of samples
- **Basis for Effort**
  - Detailed simulations of ion motion in ion traps
  - Decade-long study of ion trap performance
  - Collaboration between Purdue, Crane, and Griffin, a start-up company who will manufacture instruments

Methodology



Multiple Stages of Selectivity

- Selective Adsorption/Desorption
- Selective Ionization
- Selective Mass Analysis
- Selective Dissociation and MS/MS Analysis

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Miniaturization of the Mass Spectrometer

BEEQ – Research grade laboratory Instrument
Size: Big
Weight : 4 tons
Power : 15,000 W

Modified ITS-40 Rugged Transportable
Size: 200x 200x 100 cm
Weight: 800 lbs
Power: 4500 W

Mini-CIT Ver. 5.0
Size: 45 x 60 x 71 cm
Weight: 140 lbs
Power: 200 - 300 W

Mini-CIT Ver. 7.0
- **Size 18cm x 28cm x 65cm**
- **Weight: 60 lbs**
- **Power 120W**

Current Commercial System

Griffin Analytical Technologies

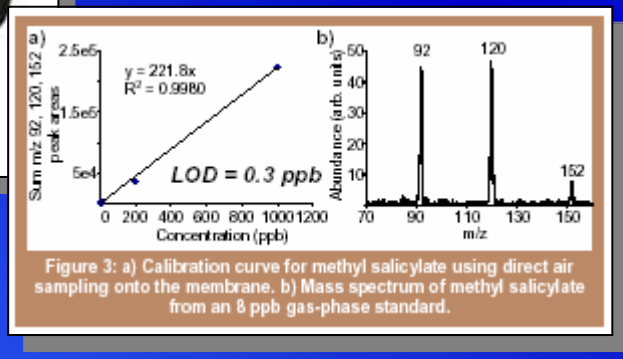
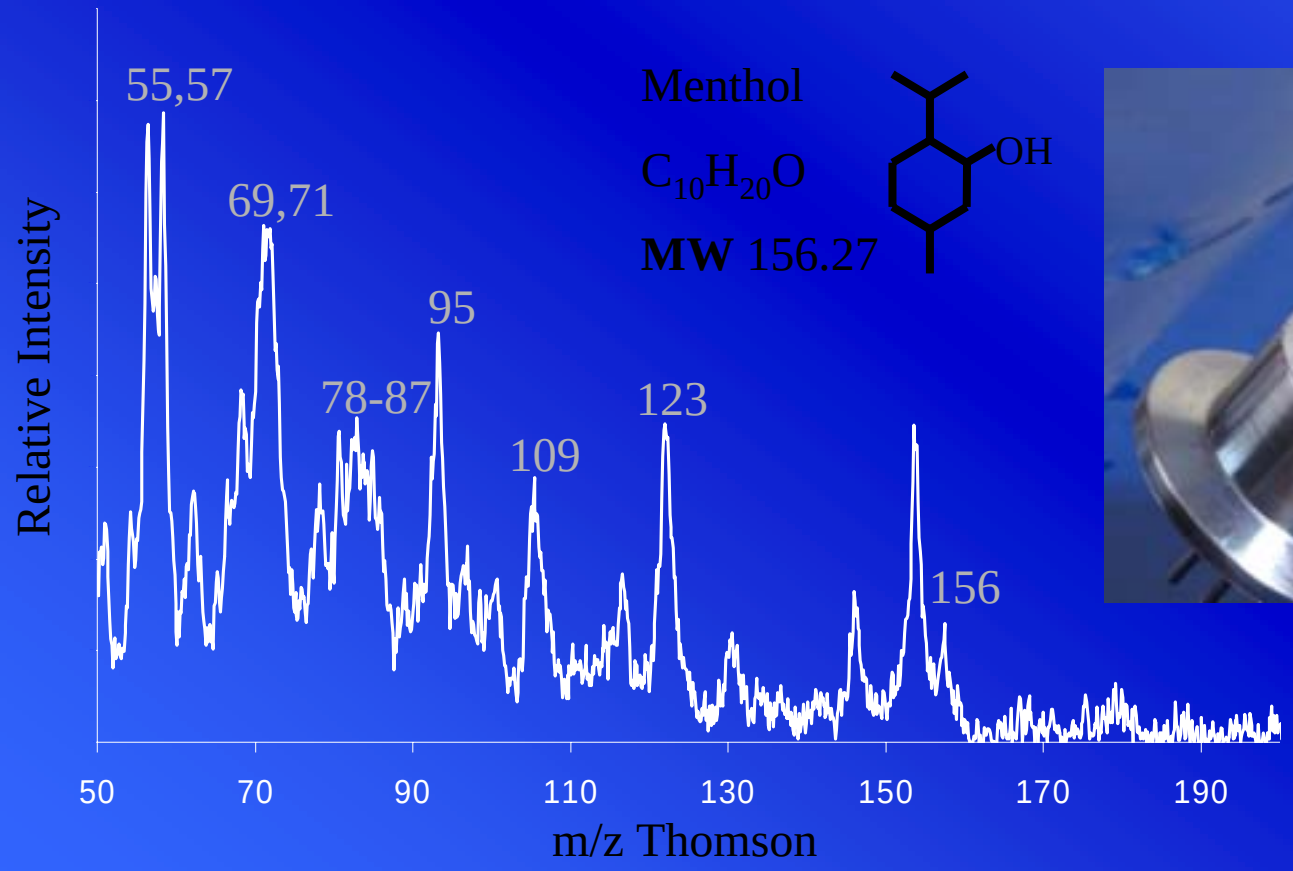


Figure 3: a) Calibration curve for methyl salicylate using direct air sampling onto the membrane. b) Mass spectrum of methyl salicylate from an 8 ppb gas-phase standard.

Mini Mass Spec Monitoring of Menthol from Cough Drops in Air

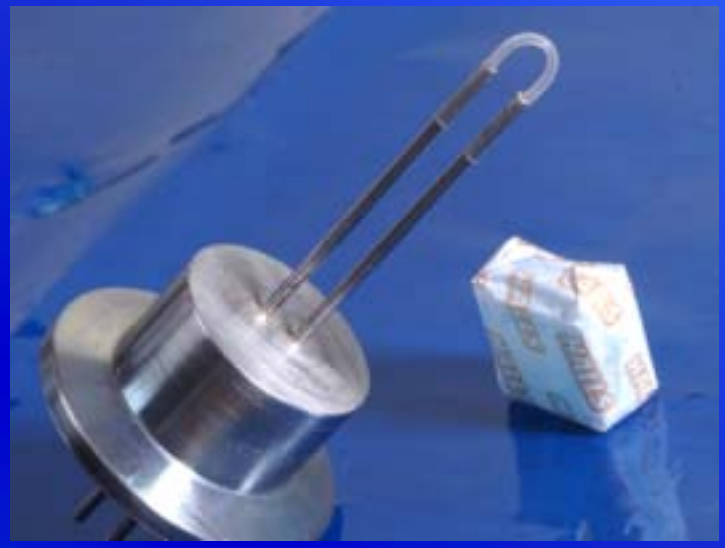
Halls cough drops (12 mg menthol per drop) in air
mini 5.0 with internal unheated membrane



Menthol

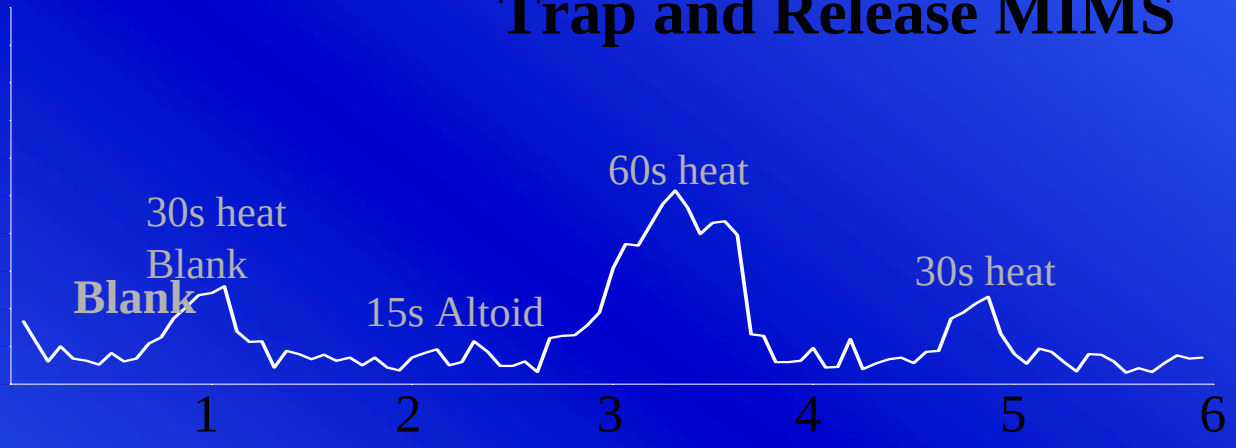
$C_{10}H_{20}O$

MW 156.27

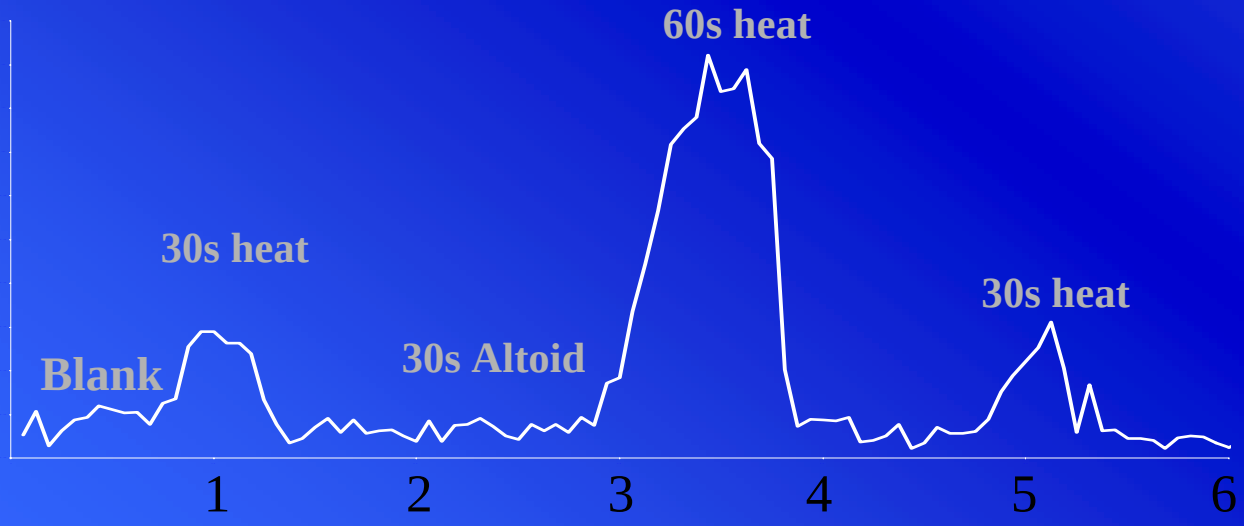


Altoid in Air: Mini Mass Spec

Trap and Release MIMS



0.45 V peak height
Rise :26 sec.
Fall: 26 sec.



0.9 V peak height
Rise :30 sec.
Fall: 30 sec.

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Membrane Introduction Test Set

- Flow-Bench with mass flow meters
- RTDs/Humidity sensors
- Variable membrane heater
- Vacuum chamber with variable pump
- Dual chamber vapor generator
- Automated testing

Mini-Mass Spectrometer

New Design

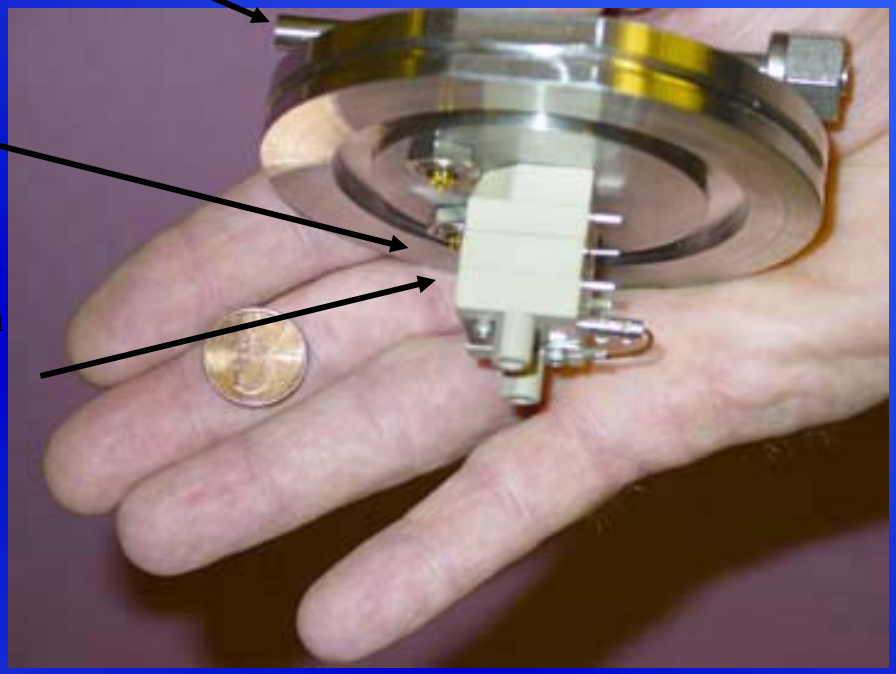
Sample Inlet

Filament

Ion Lenses

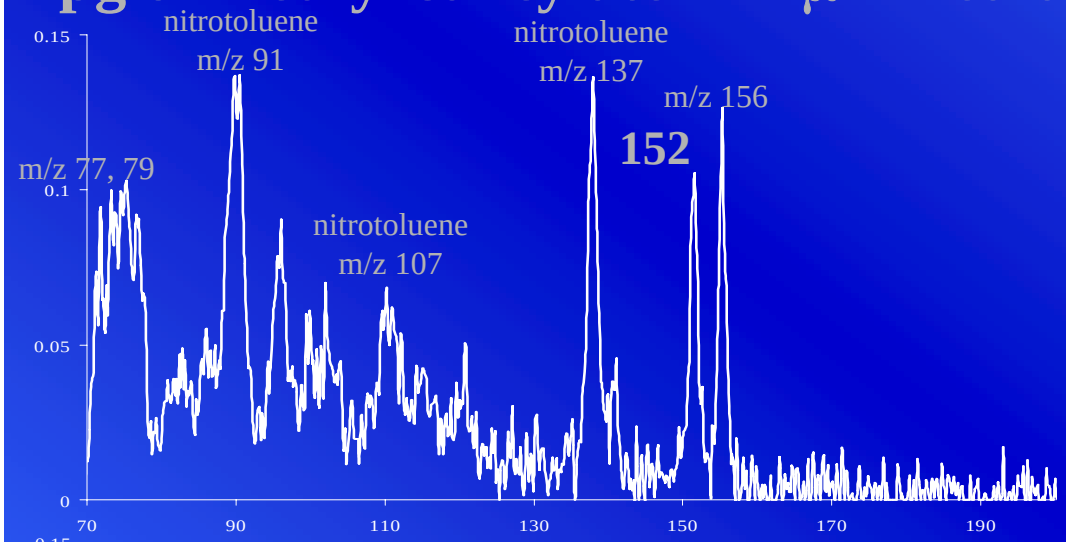
Cylindrical Ion Trap
r_0 = 2.5 mm

Current Design

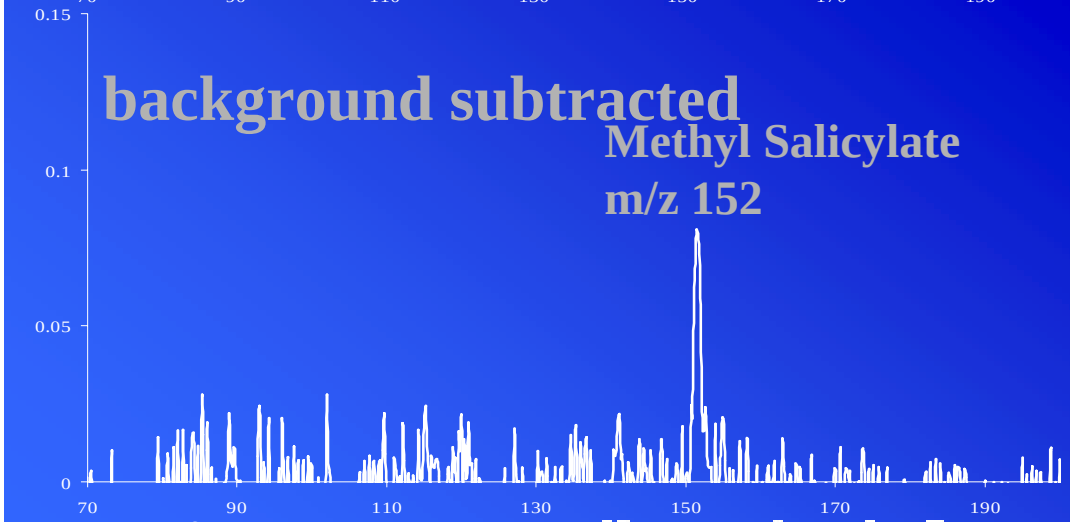


Performance Characteristics: Sensitivity and Resolution

1 pg of methyl salicylate in 1 μL methanol



Resolution ~100
Toluene with membrane inlet



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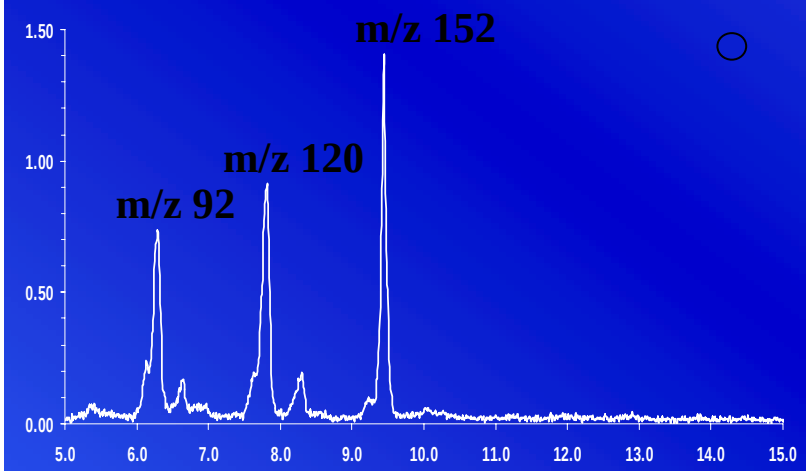
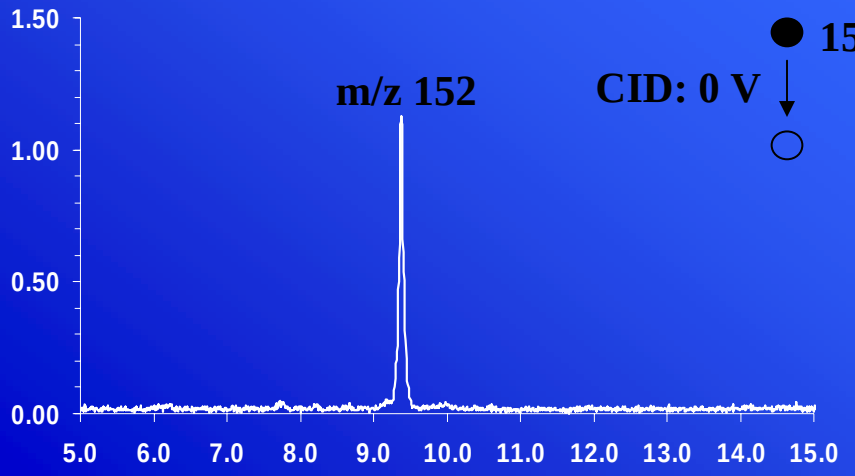
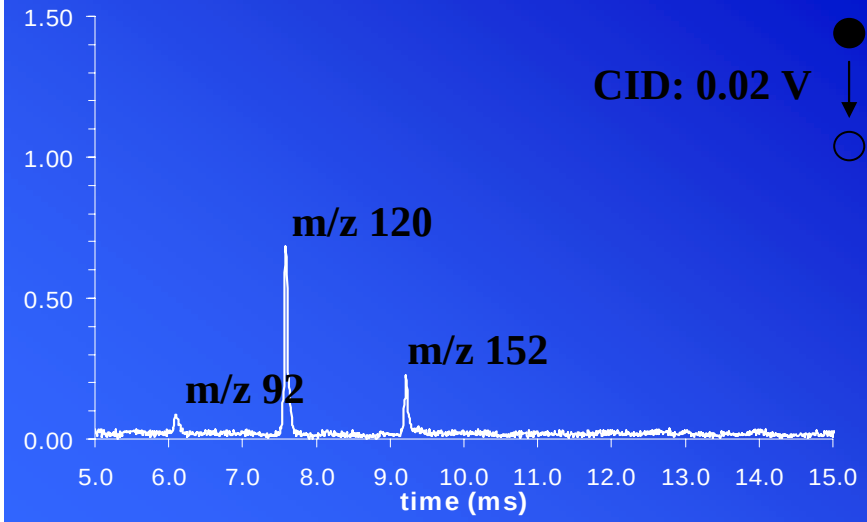
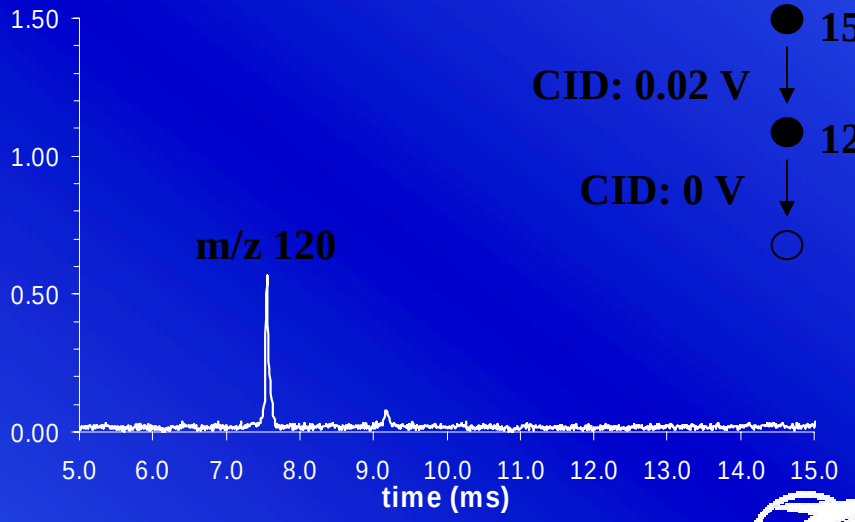
MS^n of Methyl Salicylate









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Wavelets

- Wavelet transform
  - Definition

$$WT_x(a,\tau)=\frac{1}{\sqrt{a}}\int x(t)\psi^*\left(\frac{t-\tau}{a}\right)dt$$

  - Admissible condition

$$c_\psi=\int_0^\infty\frac{|\Psi(\omega)|^2}{\omega}d\omega<\infty$$

  - Inverse transform

$$x(t)=\frac{1}{c_\psi}\int_0^\infty\frac{da}{a^2}\int_{-\infty}^{+\infty}WT_x(a,\tau)\frac{1}{\sqrt{a}}\psi\left(\frac{t-\tau}{a}\right)d\tau$$

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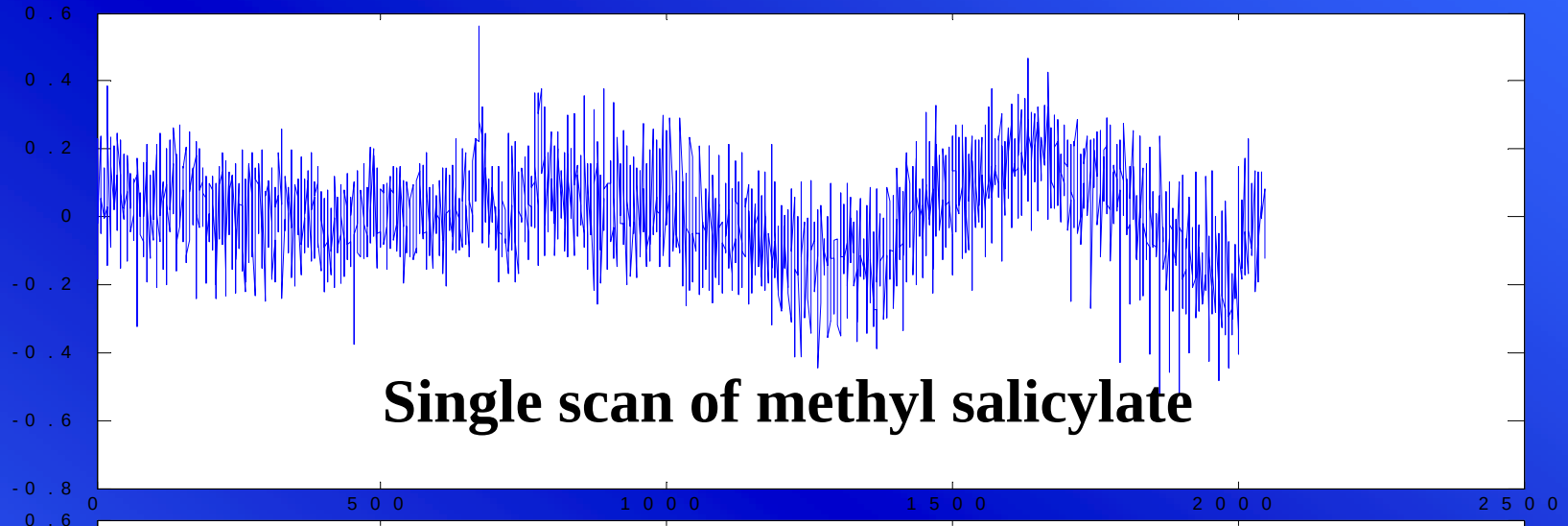
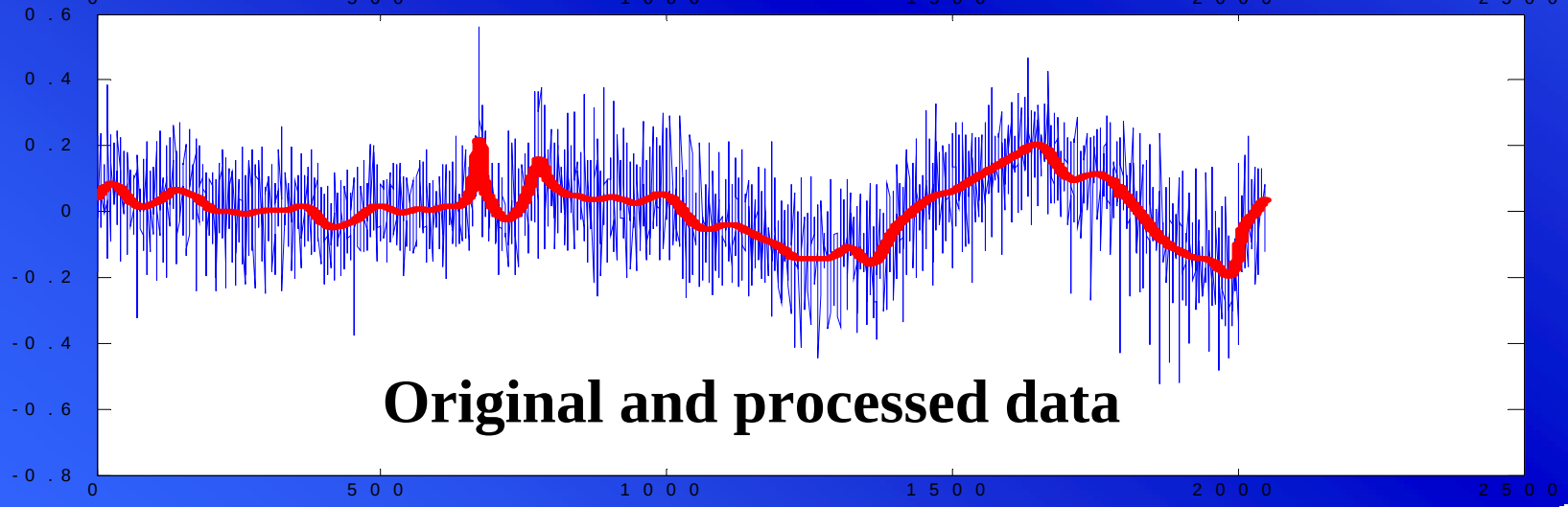
Signal Processing of Data

Wavelet Filtering



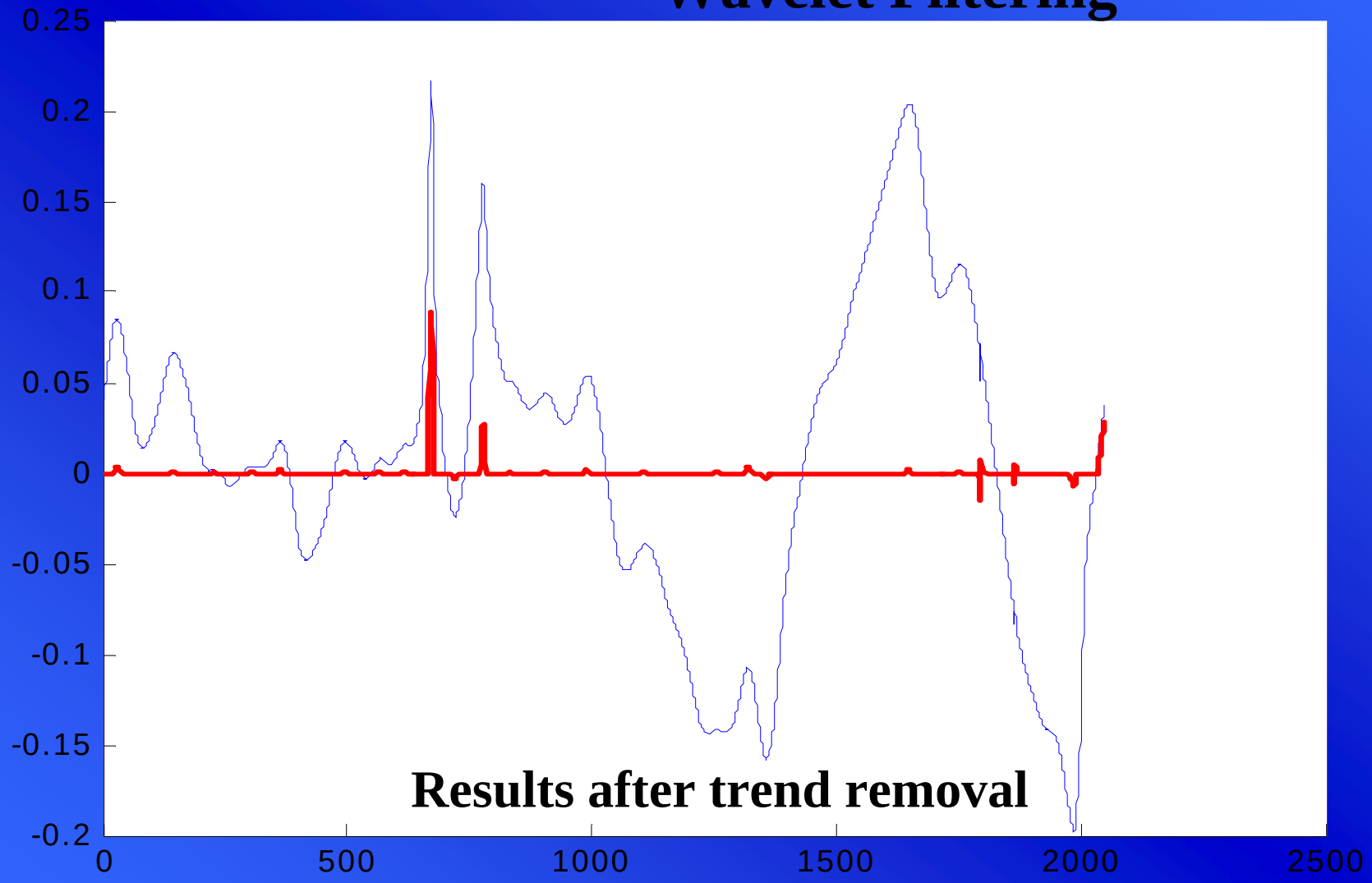
Single scan of methyl salicylate



Original and processed data

Signal Processing of Data

Wavelet Filtering



Results after trend removal

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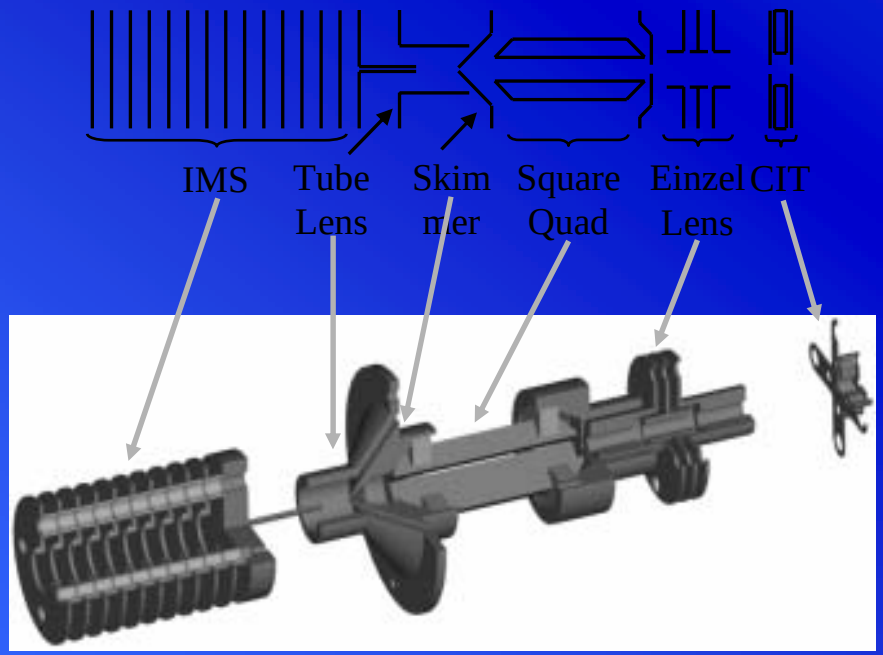
CIT Automated Test Set

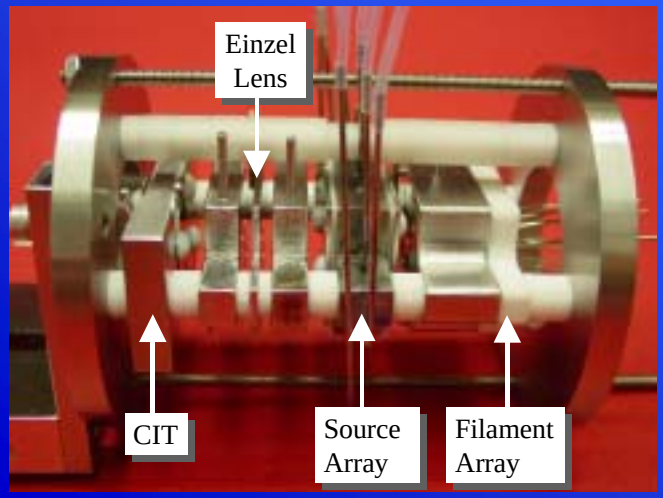
- Fully automated PXI based control system
- Control software written in LabVIEW
- Leak valve and membrane introduction system
- Couple with flow bench and vapor generator

Future Work

IMS-MS



Multiplexed CIT



- System integration
- Performance optimization
- IMS-MS
- Multiplexed CIT
- Biological Capabilities
- Algorithm Development

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